STRUCTURE AND NON-COVALENT INTERACTIONS OF THE BENZOFURAN-FORMALDEHYDE COMPLEX EXPLORED BY MICROWAVE SPECTROSCOPY AND QUANTUM-CHEMICAL CALCULATIONS

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The rotational spectrum of the benzofuran-formaldehyde complex has been investigated by high resolution Fourier transform microwave spectroscopy. In addition to the parent species, the rotational spectra of all mono-substituted ^{13}C isotopologues and the complex with $H_2C^{18}O$ have been also measured. This extensive set of rotational constants for isotopic species allowed an accurate structural determination exploiting the so-called "semi-experimental" approach.

In the observed isomer, the two subunits orient themselves almost parallel to each other. The non-covalent bonding distance between the carbon atom of formaldehyde and the nearest carbon atom of benzofuran has been found to be well within the sum of van der Waals radius of carbon. The joint experimental and computational study pointed out that the two moieties are linked through a π-π interaction. The interaction energy is calculated to be about 20 kJ mol^{-1} and, according to a SAPT analysis, is dominated by dispersion.